

Rummukainen-Gottlieb's formula on two-particle system with different mass

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Lüscher established a non-perturbative formula to extract the elastic scattering phases from two-particle energy spectrum in a torus using lattice simulations. Rummukainen and Gottlieb further extend it to the moving frame, which is devoted to the system of two identical particles. In this work, we generalize Rummukainen-Gottlieb's formula to the generic two-particle system where two particles are explicitly distinguishable, namely, the masses of the two particles are different. The finite size formula are achieved for both C_{4v} and C_{2v} symmetries. Our analytical results will be very helpful for the study of some resonances, such as kappa, vector kaon, and so on.

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I. INTRODUCTION

Many low energy hadrons, such as kappa, sigma, can be observed as resonances in the experiments. The energy eigenvalues of two-particle systems can be achieved by calculating the propagators using lattice QCD. Hence, it is highly desired to connect these calculated energy eigenstates to the experimental scattering phases. Lüscher [1–5] have established a non-perturbative formula to connect two-particle system's energy in a torus with the elastic scattering phase. Rummukainen and Gottlieb further extended Lüscher's formula to the moving frame (MF) [6]. Moreover, Xu Feng et al generalized Lüscher's formula in an asymmetric box [7]. These formulae have been employed in many different applications [8–19].

For some cases, we have to use the generic two-particle system to extract the resonance parameters in the moving frame. However, all of these aforementioned formulae in the moving frame can apply only to two identical particle system. For example, to examine the behavior of the κ resonance, it is highly desired for us to investigate πK scattering in the moving frame. For a generic two-particle system in the moving frame, we should change the Rummukainen-Gottlieb's formulae, which is devoted to the system of two identical particles. To this purpose, we will strictly derive the equivalents of the Rummukainen-Gottlieb's formulae for a generic two-particle system in the moving frame not only from theoretical aspects, but also from practical considerations. This is very helpful for the lattice study since it provides a feasible method in the study of the κ decay, vector kaon K^* decay, and so on.

The alterations of the Rummukainen-Gottlieb's formulae are mainly relevant with the different symmetries of two-particle system in a torus¹. The representations of the rotational group $O(h)$ are decoupled into irre-

ducible representations of the D_{4h} and D_{2h} cubic groups for the system of two identical particles with the non-zero total momentum in a torus [6]. In a generic two-particle system, the symmetry is reduced. For the case of $\mathbf{d} = (0, 0, 1)$, the basic group is C_{4v} instead of D_{4h} ; As for $\mathbf{d} = (0, 1, 1)$, the basic group becomes C_{2v} . Hence, the final finite size formula for the generic two-particle system in the moving frame is certainly new.

This paper is organized as follows. In Sec. II, we discuss the basic properties of the generic two-particle states in a torus. In Sec. III, we extend Rummukainen-Gottlieb's formulae to the generic case and derive the fundamental relationship for the scattering phase in Eq. (11), and in Sec. IV we present the symmetry considerations. Finally we give our brief conclusions in Sec. V.

II. GENERIC TWO-PARTICLE SYSTEM ON A CUBIC BOX

Here we derive the formalisms required for calculating the scattering phases in a cubic box, which are enough for studying lattice simulation data. However, in concrete lattice calculation, we should address the lattice artifacts [20]. In this section we follow the Rummukainen and Gottlieb's notations and conventions [6], and extend them to the generic two-particle systems.

Without loss of generality, we consider two particles with masses m_1 and m_2 for particle 1 and particle 2, respectively. In this work we are specially interested in a system having a non-zero total momentum, namely, the moving frame [6]. Using a moving frame with total momentum $\mathbf{P} = (2\pi/L)\mathbf{d}$, $\mathbf{d} \in \mathbb{Z}^3$, the energy eigenvalues for two-particle system in the non-interacting case are given by [6]

$$E_{MF} = \sqrt{m_1^2 + p_1^2} + \sqrt{m_2^2 + p_2^2},$$

where $p_1 = |\mathbf{p}_1|$, $p_2 = |\mathbf{p}_2|$, and \mathbf{p}_1 , \mathbf{p}_2 denote the three-momenta of the particle 1 and particle 2, respectively, which obey the periodic boundary condition,

$$\mathbf{p}_i = \frac{2\pi}{L}\mathbf{n}_i, \quad \mathbf{n}_i \in \mathbb{Z}^3,$$

¹ It is Naruhito Ishizuka who first help us to find the correct symmetry of the two-particle system with unequal mass. In there, we especially thank him. Without his kind help, we can not finish this work smoothly.

and the relation

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{P}. \quad (1)$$

In the center-of-mass (CM) frame, the total CM momentum disappears, namely,

$$p^* = |\mathbf{p}^*|, \quad \mathbf{p}^* = \mathbf{p}_1^* = -\mathbf{p}_2^*,$$

where $\mathbf{p}^* = (2\pi/L)\mathbf{n}$, and $\mathbf{n} \in \mathbb{Z}^3$. Here and hereafter we define the CM momenta with an asterisk (*). The possible energy eigenstates of the generic two-particle system are given by

$$E_{CM} = \sqrt{m_1^2 + p^{*2}} + \sqrt{m_2^2 + p^{*2}}.$$

The relativistic four-momentum squared is invariant, and E_{CM} is related to E_{MF} in the moving frame through the Lorentz transformation

$$E_{CM}^2 = E_{MF}^2 - \mathbf{P}^2.$$

In the moving frame, the center-of-mass is moving with a velocity of $\mathbf{v} = \mathbf{P}/E_{MF}$. Using the standard Lorentz transformation with a boost factor $\gamma = 1/\sqrt{1 - \mathbf{v}^2}$, the E_{CM} can be obtained through $E_{CM} = \gamma^{-1}E_{MF}$, and momenta \mathbf{p}_i and \mathbf{p}^* are related by the standard Lorentz transformation,

$$\mathbf{p}_1 = \vec{\gamma}(\mathbf{p}^* + \mathbf{v}E_1^*), \quad \mathbf{p}_2 = -\vec{\gamma}(\mathbf{p}^* - \mathbf{v}E_2^*), \quad (2)$$

where E_1^* and E_2^* are energy eigenvalues of the particle 1 and particle 2 in the center-of-mass frame, respectively,

$$\begin{aligned} E_1^* &= \frac{1}{2E_{CM}} (E_{CM}^2 + m_1^2 - m_2^2), \\ E_2^* &= \frac{1}{2E_{CM}} (E_{CM}^2 + m_2^2 - m_1^2), \end{aligned} \quad (3)$$

and the boost factor acts in the direction of \mathbf{v} , here and hereafter we adopt the shorthand notation

$$\vec{\gamma}\mathbf{p} = \gamma\mathbf{p}_{\parallel} + \mathbf{p}_{\perp}, \quad \vec{\gamma}^{-1}\mathbf{p} = \gamma^{-1}\mathbf{p}_{\parallel} + \mathbf{p}_{\perp}, \quad (4)$$

where \mathbf{p}_{\parallel} and \mathbf{p}_{\perp} are the \mathbf{p} components which are parallel and perpendicular to the CM velocity, respectively, namely,

$$\mathbf{p}_{\parallel} = \frac{\mathbf{p} \cdot \mathbf{v}}{|\mathbf{v}|^2} \mathbf{v}, \quad \mathbf{p}_{\perp} = \mathbf{p} - \mathbf{p}_{\parallel}. \quad (5)$$

Thus, by inspecting Eqs. (1), (2) and (3), it can be seen that the \mathbf{p}^* are quantized to the values

$$\mathbf{p}^* = \frac{2\pi}{L}\mathbf{r}, \quad \mathbf{r} \in P_{\mathbf{d}},$$

where the set $P_{\mathbf{d}}$ is

$$P_{\mathbf{d}} = \left\{ \mathbf{r} \left| \mathbf{r} = \vec{\gamma}^{-1} \left[\mathbf{n} + \frac{\mathbf{d}}{2} \cdot \left(1 + \frac{m_2^2 - m_1^2}{E_{CM}^2} \right) \right], \mathbf{n} \in \mathbb{Z}^3 \right. \right\}. \quad (6)$$

In the interacting case, the \overline{E}_{CM} is given by

$$\overline{E}_{CM} = \sqrt{m_1^2 + k^2} + \sqrt{m_2^2 + k^2}, \quad k = \frac{2\pi}{L}q. \quad (7)$$

where q is no longer required to be an integer. Solving this equation for scattering momentum k we get

$$k = \frac{1}{2\overline{E}_{CM}} \sqrt{[\overline{E}_{CM}^2 - (m_1 - m_2)^2][\overline{E}_{CM}^2 - (m_1 + m_2)^2]}. \quad (8)$$

We can rewrite Eq. (8) to an elegant form as

$$k^2 = \frac{\overline{E}_{CM}^2}{4} + \frac{(m_1^2 - m_2^2)^2}{4\overline{E}_{CM}^2} - \frac{m_1^2 + m_2^2}{2}. \quad (9)$$

It is exactly this energy shift between the non-interacting situation and interacting case, namely, $\overline{E}_{CM} - E_{CM}$ (or equivalently $|\mathbf{n}|^2 - q^2$), that we can evaluate two particle scattering phase.

As it is done in Ref. [6], in the current study, we mainly investigate two moving frames. One is $\mathbf{d} = (0, 0, 1)$, where energy eigenstates transform under the tetragonal group C_{4v} , only the irreducible representation A_1 is relevant for two-particle scattering states in a cubic box with angular momentum $l = 0$. Another one is $\mathbf{d} = (0, 1, 1)$, where energy eigenstates transform under the tetragonal group C_{2v} , only the irreducible representation A_1 is relevant. For the other cases, like $\mathbf{d} = (1, 1, 1)$, etc., we can easily work out from same way without difficulty.

Assuming that the phase shifts δ_l with $l = 1, 2, 3, \dots$ are tiny in our concerned energy range, the s -wave phase shift δ_0 is connected to the scattering momentum k by

$$\tan \delta_0(k) = \frac{\gamma \pi^{3/2} q}{\mathcal{Z}_{00}^{\mathbf{d}}(1; q^2)}, \quad (10)$$

where $k = (2\pi/L)q$, and the modified zeta function is defined by

$$\mathcal{Z}_{00}^{\mathbf{d}}(s; q^2) = \sum_{\mathbf{r} \in P_{\mathbf{d}}} \frac{1}{(|\mathbf{r}|^2 - q^2)^s}, \quad (11)$$

and the set $P_{\mathbf{d}}$ is

$$P_{\mathbf{d}} = \left\{ \mathbf{r} \left| \mathbf{r} = \vec{\gamma}^{-1} \left[\mathbf{n} + \frac{\mathbf{d}}{2} \cdot \left(1 + \frac{m_2^2 - m_1^2}{E_{CM}^2} \right) \right], \mathbf{n} \in \mathbb{Z}^3 \right. \right\}. \quad (12)$$

For Eq. (10), we note that the almost same result has already existed in Eq. (1) of Ref. [21], where the formula was just presented without any explanation. We can view our work as further confirming and strictly proving this formula. The modified zeta function converges when $\text{Re } 2s > l + 3$, and it can be analytically continued to whole complex plane. The scattering momentum k is defined from the invariant mass \sqrt{s} as $\sqrt{s} = \overline{E}_{CM} = \sqrt{k^2 + m_1^2} + \sqrt{k^2 + m_2^2}$. The calculation method of $\mathcal{Z}_{00}^{\mathbf{d}}(1; q^2)$ is discussed in Appendix A and in Ref. [20]. Using Eq. (10), we can obtain the phase shift from the energy spectrum using lattice simulations. If we now set $m_1 = m_2$, all the results in Ref. [6] are elegantly recovered.

III. DERIVATION OF THE PHASE SHIFT FORMULA

Here we deduce the basic phase shift formula in Eq. (10) for the generic two-particle system with spin-0. We utilize the Rummukainen and Gottlieb's formulae in Ref. [6], and extend them to the generic two-particle system. To make the derivation simple, we are studying the system by the relativistic quantum mechanics.

Throughout this section, we employ the metric tensor sign convention $g_{\mu\nu} = \text{diag}(1, -1, -1, -1)$, write the scalar products in a compact form $p^2 = p \cdot p = p_\mu p^\mu$, etc, and express the quantities in natural units with $\hbar = c = 1$. Here and hereafter we follow the original notations in Refs. [6].

A. Lorentz transformation of wave function

Let us consider the generic system of two spin-0 particles with mass m_1 , and m_2 , respectively, in a cubic box. The two-particle system is described by the scalar wave function $\psi(x_1, x_2)$, where $x_i = (x_i^0, \mathbf{x}_i)$, $i = 1, 2$ are the four-dimensional Minkowski coordinates of two particles. The wave function changes under the standard Lorentz transformations, namely,

$$\psi(x_1, x_2) = \psi'(x'_1, x'_2) = \psi'(\Lambda x_1, \Lambda x_2), \quad (13)$$

where $(x')^\mu = \Lambda^\mu_\nu x^\nu$ defines the standard Lorentz transformation of the four-vector x .

We can make the problem easier through the special properties of the CM frame. First let us study two non-interacting particles, and the wave functions of the system obey the Klein-Gordon (KG) equations

$$\begin{aligned} (\hat{p}_{1\mu} \hat{p}_1^\mu - m_1^2) \psi(x_1, x_2) &= 0, \\ (\hat{p}_{2\mu} \hat{p}_2^\mu - m_2^2) \psi(x_1, x_2) &= 0, \end{aligned} \quad (14)$$

where $\hat{p}_{i\mu}$, $i = 1, 2$ is the four-momentum operator. It is well-known, the problem simplifies if we separate the variables under the transformations

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}, \quad (15)$$

$$x = x_1 - x_2, \quad (16)$$

where X is the position of the CM, and x is the relative coordinate of two particles. Let us restrict ourselves to the solutions which are the eigenstates of the CM momentum operator. Then Eq. (14) can be changed into

$$\left[\frac{m_1^2}{M^2} \hat{P}_\mu \hat{P}^\mu + \hat{p}_\mu \hat{p}^\mu - \frac{2m_1}{M} \hat{p}_\mu \cdot \hat{P}^\mu + m_1^2 \right] \psi(x, X) = 0, \quad (17)$$

$$\left[\frac{m_2^2}{M^2} \hat{P}_\mu \hat{P}^\mu + \hat{p}_\mu \hat{p}^\mu + \frac{2m_2}{M} \hat{p}_\mu \cdot \hat{P}^\mu + m_2^2 \right] \psi(x, X) = 0, \quad (18)$$

where

$$\hat{p} = \frac{m_2 \hat{p}_1 - m_1 \hat{p}_2}{m_1 + m_2}, \quad (19)$$

$$\hat{P} = \hat{p}_1 + \hat{p}_2, \quad (20)$$

$$M = m_1 + m_2, \quad (21)$$

\hat{p} is relative four-momentum operator, \hat{P} is total four-momentum operator, and M is total mass of two particles. Adding $1/m_1 \times (17)$ to $1/m_2 \times (18)$ and subtracting (17) from (18), respectively, yield

$$\left[\frac{M^2}{m_1 m_2} \hat{p}_\mu \hat{p}^\mu - M^2 + \hat{P}_\mu \hat{P}^\mu \right] \psi(x, X) = 0, \quad (22)$$

$$\left[\hat{p}_\mu \hat{P}^\mu - \frac{m_1 - m_2}{2M} \hat{P}_\mu \hat{P}^\mu - \frac{m_1^2 - m_2^2}{2} \right] \psi(x, X) = 0. \quad (23)$$

It is well-known that, without external potentials, the total momentum of the two-particle system is conserved, thus we can restrain ourselves to the eigenfunctions of P , namely,

$$\psi(x, X) = e^{-iP_\mu X^\mu} \phi(x), \quad (24)$$

where P_μ is a constant time-like vector, and P is denoted through $P^2 = P_\mu P^\mu$.

In the present study, we are specially interested in the CM frame, which is denoted as the frame without the spatial components of the total momentum for the system, namely, $\mathbf{P}^* = 0$. Thus, we can only take the positive kinetic energy solutions $P_0^* = E_{\text{CM}}^* > m_1 + m_2$ into consideration. So, Eqs. (22) and (23) can be rewritten as,

$$\left(\hat{p}_\mu^* \hat{p}^{*\mu} + \frac{E_{\text{CM}}^* m_1 m_2}{(m_1 + m_2)^2} - m_1 m_2 \right) \phi_{\text{CM}}(x^*) = 0, \quad (25)$$

$$\left(\hat{p}_0^* - \frac{E_{\text{CM}}}{2} \frac{m_1 - m_2}{m_1 + m_2} - \frac{m_1^2 - m_2^2}{2E_{\text{CM}}} \right) \phi_{\text{CM}}(x^*) = 0. \quad (26)$$

Eq. (26) indicates $\hat{p}_0^* \phi_{\text{CM}}(x^*) \neq 0$ for $m_1 \neq m_2$. By inspecting Eq. (25) and Eq. (26), we can reasonably assume that the wave function $\phi_{\text{CM}}(x^*)$ can be expressed as

$$\phi_{\text{CM}}(x^*) \equiv e^{i\beta x^{*0}} \phi_{\text{CM}}(\mathbf{x}^*), \quad (27)$$

where $x^{*0} = x_1^{*0} - x_2^{*0}$ is the relative temporal separation of two particles, and β is a constant, namely,

$$\beta = \frac{E_{\text{CM}}}{2} \frac{m_2 - m_1}{m_1 + m_2} + \frac{m_2^2 - m_1^2}{2E_{\text{CM}}}. \quad (28)$$

It is obvious that when $m_1 = m_2$, $\beta \rightarrow 0$. So, in the CM frame the wave function depends explicitly on the time variable $t^* \equiv X^{*0} = (m_1 x_1^{*0} + m_2 x_2^{*0})/(m_1 + m_2)$, the relative spatial separation $\mathbf{x}^* = \mathbf{x}_1^* - \mathbf{x}_2^*$, and the relative temporal separation of the particles x^{*0} , namely,

$$\psi_{\text{CM}}(x^*, t^*) = e^{-iE_{\text{CM}} t^*} e^{i\beta x^{*0}} \phi_{\text{CM}}(\mathbf{x}^*), \quad (29)$$

where the constant β is denoted in Eq. (28).

Now let us discuss the case in the moving frame. The transformation from the MF to CM frame can be expressed as $r^{*\mu} = \Lambda^\mu_\nu r^\nu$, where r is any position four-vector and quantities without * stand for these in the moving frame. Using the notation in (4), we have

$$r^{*0} = \gamma(r^0 + \mathbf{v} \cdot \mathbf{r}), \quad \mathbf{r}^* = \vec{\gamma}(\mathbf{r} + \mathbf{v}r^0), \quad (30)$$

where γ is a boost factor, and $\mathbf{v} = \mathbf{P}/P_0$ is the three-velocity of the CM in the moving frame. We can rewrite \mathbf{v} to a form for later use as

$$\mathbf{v} = \frac{2\pi}{LE_{\text{MF}}} \mathbf{d} = \frac{2\pi}{\gamma LE_{\text{CM}}} \mathbf{d}. \quad (31)$$

Considering the identity $P_\mu X^\mu = P_\mu^* X^{*\mu}$, the Lorentz transformation in Eq. (13), and Eq. (24), the wave function in the moving frame can be expressed as

$$\psi_{\text{MF}}(x, X) = e^{-iP_\mu X^\mu} \phi_{\text{MF}}(x),$$

where

$$\phi_{\text{MF}}(x) \equiv \phi_{\text{MF}}(x^0, \mathbf{x}) = \phi_{\text{CM}}(\gamma(x^0 + \mathbf{v} \cdot \mathbf{x}), \vec{\gamma}(\mathbf{x} + \mathbf{v}x^0)). \quad (32)$$

Thus, the wave function ϕ_{MF} depends on time separation $x^0 = x_1^0 - x_2^0$ explicitly. However, in the moving frame we only consider two particles with the same time coordinate, namely, $x^0 = 0$. It corresponds to the tilted plane $(x^{*0}, \mathbf{x}^*) = (\gamma \mathbf{v} \cdot \mathbf{x}, \vec{\gamma} \mathbf{x})$ for the CM frame, since the wave function ϕ_{CM} is dependent of the relative temporal separation x^{*0} , we can clearly observe the effect of the tilt to the wave function, and Eq. (32) take as

$$\phi_{\text{MF}}(0, \mathbf{x}) = \phi_{\text{CM}}(\gamma \mathbf{v} \cdot \mathbf{x}, \vec{\gamma} \mathbf{x}). \quad (33)$$

Using Eq. (27) and Eq. (31), we can rewrite Eq. (33) as

$$\phi_{\text{MF}}(0, \mathbf{x}) = e^{i\beta' \pi \mathbf{d} \cdot \mathbf{x}/L} \phi_{\text{CM}}(\vec{\gamma} \mathbf{x}). \quad (34)$$

where β' is a constant, namely,

$$\beta' = \frac{m_2 - m_1}{m_1 + m_2} + \frac{m_2^2 - m_1^2}{E_{\text{CM}}^2}. \quad (35)$$

Eq. (34) has a simple physical meaning: the CM system watches the torus in the moving frame expanded by a boost factor γ in the direction of \mathbf{P} , and the length scales in perpendicular directions are hold. At last, Eq. (34) connects the MF wave function,

$$\psi_{\text{MF}}(0, \mathbf{x}, t, \mathbf{X}) = e^{-iE_{\text{MF}}t + i\mathbf{P} \cdot \mathbf{X}} \phi_{\text{MF}}(0, \mathbf{x}), \quad (36)$$

to the CM frame wave function Eq. (29). By inspecting Eqs. (25), (26) and (29), we, at last, achieve the wave function ϕ_{CM} meeting the Helmholtz equation (HE)

$$(\nabla_{\mathbf{x}^*}^2 + k^{*2}) \phi_{\text{CM}}(\mathbf{x}^*) = 0, \quad (37)$$

where

$$k^{*2} = \frac{E_{\text{CM}}^2}{4} + \frac{(m_1^2 - m_2^2)^2}{4E_{\text{CM}}^2} - \frac{m_1^2 + m_2^2}{2}. \quad (38)$$

This result is consistent with the solution in Ref. [22].

The Eqs. (34) and (37) are very important when we study the wave functions of our system. Thus Eq. (37) is a very important result, which represents one of the main results of the present work. In the following studies, we take away the superscript * from the quantities in the CM frame. We can easily check that if we take $m_1 = m_2$, all the corresponding results in Ref. [6] are restored.

B. Modified singular d-periodic solutions of the Helmholtz equation

In our concrete problem, for the potential $V_\mu(\mathbf{x})$ with a limit range [2], namely,

$$V_\mu(\mathbf{x}) = 0 \quad \text{for } |\mathbf{x}| > R, \quad (39)$$

we suppose that the KG equation (14) in the CM frame still has a square integral solution. In the CM frame the interaction of the system is spherically symmetric. The wave function of the system is usually given in spherical harmonics

$$\phi_{\text{CM}}(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\theta, \varphi) \phi_{lm}(x). \quad (40)$$

For $x > R$, ϕ_{CM} is a solution of HE, and the radial functions ϕ_{lm} meet the differential equation

$$\left[\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} - \frac{l(l+1)}{x^2} + k^2 \right] \phi_{lm}(x) = 0, \quad (41)$$

where

$$k^2 = \frac{E_{\text{CM}}^2}{4} + \frac{(m_1^2 - m_2^2)^2}{4E_{\text{CM}}^2} - \frac{m_1^2 + m_2^2}{2}. \quad (42)$$

With the linear combinations of the spherical Bessel functions the solutions of Eq. (41) can be expressed as

$$\phi_{lm}(x) = c_{lm} [a_l(k) j_l(kx) + b_l(k) n_l(kx)]. \quad (43)$$

Although we do not know the radial equation in the region $x < R$, by comparing the wave functions denoted in Eqs. (40,43), we can get the relation between the scattering phase and the coefficients a_l and b_l [2], namely,

$$e^{i2\delta_l(k)} = \frac{a_l(k) + ib_l(k)}{a_l(k) - ib_l(k)}.$$

Because the radial equation a_l and b_l can be taken to be the real number for $k > 0$, $\delta_l(k)$ is real. Thus, for a given l -sector, the phase shift $\delta_l(k)$ can be expressed by energy E_{MF} through

$$k^2 = \frac{E_{\text{MF}}^2 - \mathbf{P}^2}{4} + \frac{1}{4} \frac{(m_1^2 - m_2^2)^2}{E_{\text{MF}}^2 - \mathbf{P}^2} - \frac{m_1^2 + m_2^2}{2}.$$

In the moving frame, we now investigate two generic particles confined in a torus of size L^3 with periodic

boundary conditions(PBC). The temporal direction of the torus is chosen to be infinite. The wave functions ψ_{MF} in MF should be periodic with regard to the position of each particle, namely,

$$\psi_{\text{MF}}(\mathbf{x}_1, \mathbf{x}_2) = \psi_{\text{MF}}(\mathbf{x}_1 + \mathbf{l}L, \mathbf{x}_2 + \mathbf{m}L), \quad \mathbf{l}, \mathbf{m} \in \mathbb{Z}^3. \quad (44)$$

The wave function ψ_{MF} is provided by (36), namely

$$\psi_{\text{MF}}(\mathbf{x}_1, \mathbf{x}_2) = \exp\left(i \frac{\mathbf{P} \cdot (m_1 \mathbf{x}_1 + m_2 \mathbf{x}_2)}{m_1 + m_2}\right) \phi_{\text{MF}}(\mathbf{x}_1 - \mathbf{x}_2). \quad (45)$$

Combining Eq. (44) and Eq. (45) gives

$$\mathbf{P} = \frac{2\pi}{L} \mathbf{d}, \quad (46)$$

$$\phi_{\text{MF}}(\mathbf{x}) = e^{i\pi \frac{2m_1}{m_1+m_2} \mathbf{d} \cdot \mathbf{n}} \phi_{\text{MF}}(\mathbf{x} + \mathbf{n}L), \quad (47)$$

where $\mathbf{n} = \mathbf{l} - \mathbf{m}$, $\mathbf{d}, \mathbf{n} \in \mathbb{Z}^3$ and \mathbf{P} is the total momentum ². The rule (47) separates the wave functions into the different sectors, which can be categorized by the three-vector \mathbf{d} . In the current study, we naturally concentrate on sectors $\mathbf{d} = (0, 0, 1)$ and $\mathbf{d} = (0, 1, 1)$.

We are now on the position to employ Eq. (34) to get the corresponding periodic rule for the CM wave function. For a chosen vector \mathbf{d} , we have

$$\phi_{\text{CM}}(\mathbf{x}) = e^{i\pi \mathbf{d} \cdot \mathbf{n} \left(1 + \frac{m_2^2 - m_1^2}{E_{\text{CM}}^2}\right)} \phi_{\text{CM}}(\mathbf{x} + \vec{\gamma} \mathbf{n}L), \quad \mathbf{n} \in \mathbb{Z}^3. \quad (48)$$

For simpleness, we refer to the functions obeying the periodicity rule (48) as modified \mathbf{d} -periodic rule. As shown later, the modified \mathbf{d} -periodic rule (48) is a milestone in this work.

Now we deduce the general solutions of the HE satisfying the modified \mathbf{d} -periodic rule (48). Except the modified \mathbf{d} -periodicity, our derivation follows the works in section 4.4 of Ref. [6]. In this work, we will refer to a function ϕ as a singular modified \mathbf{d} -periodic solution of the HE, if it is a smooth function denoted for all $\mathbf{x} \neq \vec{\gamma} \mathbf{n}L$, $\mathbf{n} \in \mathbb{Z}^3$, and it meets the HE, namely,

$$(\nabla^2 + k^2)\phi(\mathbf{x}) = 0,$$

for $k > 0$, and meets the modified \mathbf{d} -periodic rule,i.e.,

$$\phi(\mathbf{x}) = e^{i\alpha\pi \mathbf{d} \cdot \mathbf{n}} \phi(\mathbf{x} + \vec{\gamma} \mathbf{n}L), \quad \mathbf{n} \in \mathbb{Z}^3, \quad (49)$$

here and hereafter, for compactness, we defined a factor α , namely,

$$\alpha \equiv 1 + \frac{m_2^2 - m_1^2}{E_{\text{CM}}^2}. \quad (50)$$

² Eq. (47) can also be written as

$$\phi_{\text{MF}}(\mathbf{x}) = e^{-i\pi \frac{2m_2}{m_1+m_2} \mathbf{d} \cdot \mathbf{n}} \phi_{\text{MF}}(\mathbf{x} + \mathbf{n}L).$$

Following the almost same procedures and addressing the corresponding formulae, we can arrive at the same final numerical results. For our case, $\mathbf{d} \cdot \mathbf{n}$ is an integer.

When $m_1 = m_2$, $\alpha = 1$, this is the case Rummukainen and Gottlieb studied in Ref. [6]. Moreover, the wave function is required to be bounded by a power of $1/|\mathbf{x}|$ around the origin, namely

$$\lim_{\mathbf{x} \rightarrow 0} |\mathbf{x}^{\Lambda+1} \phi(\mathbf{x})| < \infty$$

for the positive integer Λ , the degree of ϕ . For our aim, it is enough to study the regular values of k , namely

$$k \neq \frac{2\pi}{L} \left| \vec{\gamma}^{-1} \left(\mathbf{n} + \frac{\alpha}{2} \mathbf{d} \right) \right|, \quad \mathbf{n} \in \mathbb{Z}^3.$$

We denote the Green function

$$G^{\mathbf{d}}(\mathbf{x}; k) = \gamma^{-1} L^{-3} \sum_{\mathbf{p} \in \Gamma} \frac{e^{i\mathbf{p} \cdot \mathbf{x}}}{\mathbf{p}^2 - k^2}, \quad (51)$$

where

$$\Gamma = \left\{ \mathbf{p} \in \mathbb{R}^3 \mid \mathbf{p} = \frac{2\pi}{L} \vec{\gamma}^{-1} \left(\mathbf{n} + \frac{\alpha}{2} \mathbf{d} \right), \quad \mathbf{n} \in \mathbb{Z}^3 \right\}.$$

Eq. (51) is well-defined due to the non-singular k . If we select $\mathbf{k} = (2\pi/L) \vec{\gamma}^{-1} (\mathbf{m} + \frac{\alpha}{2} \mathbf{d})$, $\mathbf{m} \in \mathbb{Z}^3$, then

$$\mathbf{k} \cdot (\mathbf{x} + \vec{\gamma} \mathbf{n}L) = \mathbf{k} \cdot \mathbf{x} + \alpha \pi \mathbf{d} \cdot \mathbf{n} + 2\pi \mathbf{m} \cdot \mathbf{n},$$

where $\mathbf{n} \in \mathbb{Z}^3$, and the Green function $G^{\mathbf{d}}(\mathbf{x}; k)$ meets clearly the modified \mathbf{d} -periodic rule, as we expected. Furthermore, it obeys

$$(\nabla^2 + k^2) G^{\mathbf{d}}(\mathbf{x}; k) = - \sum_{\mathbf{n} \in \mathbb{Z}^3} e^{i\alpha\pi \mathbf{d} \cdot \mathbf{n}} \delta(\mathbf{x} + \vec{\gamma} \mathbf{n}L).$$

We can easily verify that the function $G^{\mathbf{d}}(\mathbf{x}; k)$ is a singular modified \mathbf{d} -periodic solution of Helmholtz equation with degree 1. Other singular periodic solutions can be easily achieved by differentiating $G^{\mathbf{d}}$ with \mathbf{x} . And

$$G_{lm}^{\mathbf{d}}(\mathbf{x}; k) = \mathcal{Y}_{lm}(\nabla) G^{\mathbf{d}}(\mathbf{x}; k), \quad (52)$$

where the harmonic polynomials $\mathcal{Y}_{lm}(\mathbf{x}) = x^l Y_{lm}(\theta, \varphi)$. We can easily verify that the functions $G_{lm}^{\mathbf{d}}$ are singular modified \mathbf{d} -periodic solutions of the HE, and they make up a complete set of solutions so that any singular modified \mathbf{d} -periodic solution of degree Λ is just a linear combination of $G_{lm}^{\mathbf{d}}(\mathbf{x}; p)$ for $l \leq \Lambda$ [2]. In the region $0 < x < L/2$ the functions $G_{lm}^{\mathbf{d}}$ can be expanded in usual spherical harmonics, namely

$$G_{lm}^{\mathbf{d}}(\mathbf{x}; k) = \frac{(-1)^l k^{l+1}}{4\pi} [n_l(kx) Y_{lm}(\theta, \varphi) + \sum_{l'=0}^{\infty} \sum_{m'=-l}^l \mathcal{M}_{lm, l'm'}^{\mathbf{d}}(k) j_{l'}(kx) Y_{l'm'}(\theta, \varphi)]. \quad (53)$$

The regular part has the coefficients $\mathcal{M}_{lm, l'm'}^{\mathbf{d}}(k)$. In the concrete calculation, only a few of them is needed, and we also provide its general expression, namely,

$$\mathcal{M}_{lm, l'm'}^{\mathbf{d}}(k) = \frac{(-1)^l}{\gamma \pi^{3/2}} \sum_{j=|l-l'|}^{l+l'} \sum_{s=-j}^j \frac{i^j}{q^{j+1}} \mathcal{Z}_{js}^{\mathbf{d}}(1; q^2) C_{lm, js, l'm'}. \quad (54)$$

where $q = kL/(2\pi)$. Using Wigner 3j-symbols [23] the tensor $C_{lm,js,l'm'}$ can be expressed as

$$C_{lm,js,l'm'} = (-1)^{m'} i^{l-j+l'} \sqrt{(2l+1)(2j+1)(2l'+1)} \times \begin{pmatrix} l & j & l' \\ m & s & -m' \end{pmatrix} \begin{pmatrix} l & j & l' \\ 0 & 0 & 0 \end{pmatrix}. \quad (55)$$

The modified zeta function is formally denoted by

$$\mathcal{Z}_{lm}^{\mathbf{d}}(s; q^2) = \sum_{\mathbf{r} \in P_{\mathbf{d}}} \frac{\mathcal{Y}_{lm}(\mathbf{r})}{(\mathbf{r}^2 - q^2)^s}, \quad (56)$$

where

$$P_{\mathbf{d}} = \left\{ \mathbf{r} \in \mathbf{R}^3 \mid \mathbf{r} = \vec{\gamma}^{-1} \left(\mathbf{n} + \frac{\alpha}{2} \mathbf{d} \right), \quad \mathbf{n} \in \mathbb{Z}^3 \right\}.$$

In Table I we summarized the expressions of $\mathcal{M}_{lm,l'm'}^{\mathbf{d}}$ for $l, l' \leq 3$. For compactness, we denoted

$$w_{lm} = \frac{1}{\pi^{3/2} \sqrt{2l+1}} \gamma^{-1} q^{-l-1} \mathcal{Z}_{lm}^{\mathbf{d}}(1; q^2). \quad (57)$$

The Wigner 3j-symbol values can be obtained in Ref. [23]. We can easily verify that, if we set $m_1 = m_2$, all of the above definitions and formulae nicely reduce to the those obtained in Ref. [6], as we expected. Of course, if we further select $\mathbf{d} = 0$, the moving frame and the CM frame coincide, $\gamma \rightarrow 1$ and $P_{\mathbf{d}} \rightarrow \mathbb{Z}^3$, and they further neatly reduce to that in Ref. [2]. The Table I can be compared with the Table 3 in Ref. [6], which summaries the matrix elements for $m_1 = m_2$. We should stress that the functions w_{10} , w_{30} and w_{50} appear in Table I. If we set $m_1 = m_2$, then $w_{10} \rightarrow 0$, $w_{30} \rightarrow 0$, and $w_{50} \rightarrow 0$, and Rummukainen-Gottlieb's results is elegantly restored.

So far, we can arrive at

$$\begin{aligned} \sum_{l=0}^{\Lambda} \sum_{m=-l}^l v_{lm} G_{lm}^{\mathbf{d}}(\mathbf{x}, k^2) &= \\ \sum_{l=0}^{\Lambda} \sum_{m=-l}^l c_{lm} [a_l(k) j_l(kx) + b_l(k) n_l(kx)] Y_{lm}(\theta, \varphi) \end{aligned} \quad (58)$$

for the constants c_{lm} and v_{lm} . And we obtain

$$c_{lm} a_l(k) = \sum_{l'=0}^{\Lambda} \sum_{m'=-l'}^{l'} c_{l'm'} b_{l'}(k) \mathcal{M}_{l'm',lm}^{\mathbf{d}}(k). \quad (59)$$

$\mathcal{M}_{l'm',lm}^{\mathbf{d}}$ can be viewed as the matrix element of the operator M . We can express Eq. (59) as a matrix equation, $C(A - BM) = 0$, where matrix $A_{(lm),(l'm')} = a_l(p) \delta_{l,l'} \delta_{m,m'}$ (similar for B). We can denote the phase shift matrix [2, 6],

$$e^{2i\delta} = \frac{A + iB}{A - iB}.$$

The determinant condition arrives at [6]

$$\det [e^{2i\delta}(M - i) - (M + i)] = 0. \quad (60)$$

IV. SYMMETRY DISCUSSIONS

When the moving and CM frames coincide, the two-particle system has a cubic symmetry and the wave functions transforms under the representations of the cubic group O_h . On the other hand, according to Eq. (34), if two frames are not equivalent, the Lorentz translation boost from the moving frame to the CM frame and only some subgroups of O_h group survive [6].

In this work, we are mainly interested in a boost along one of the coordinate axes, namely $\mathbf{d} = (0, 0, 1)$. The geometry of the torus transforms as $(1, 1, 1) \rightarrow (1, 1, \gamma)$, and the corresponding symmetry group is tetragonal point group C_{4v} , which has 8 elements: 4 rotations through an angle $(n\pi/2)$, where $n = 0, 1, 2, 3$, around the x_3 -axis; and all four of the above multiplied by the reflection with respect to the $(1, 3)$ -plane. The relevant point groups and the boost vectors are classified in Table II.

In this work we mainly discuss the cubic and tetragonal symmetry groups O_h , C_{4v} , and C_{2v} . The tetragonal group C_{4v} has four 1-dimensional representations A_1 , A_2 , B_1 , B_2 , and one 2-dimensional representation E [24]. The representations of the rotational group are reduced into irreducible representations of C_{4v} as:

$$\begin{aligned} \Gamma^{(0)} &= A_1, \\ \Gamma^{(1)} &= A_1 \oplus E, \\ \Gamma^{(2)} &= A_1 \oplus B_1 \oplus B_2 \oplus E. \end{aligned} \quad (61)$$

The representations can be obtained through the character tables [24] or by enumerating harmonic polynomials of degree l which transform under the representations of C_{4v} . The basis polynomials for the corresponding representations are summarized in Table III for $l \leq 2$.

The tetragonal group C_{2v} has four 1-dimensional representations A_1 , A_2 , B_1 , B_2 [24]. The representations of the rotational group are further reduced into irreducible representations of C_{2v} as:

$$\begin{aligned} \Gamma^{(0)} &= A_1, \\ \Gamma^{(1)} &= A_1 \oplus B_1 \oplus B_2, \\ \Gamma^{(2)} &= A_1 \oplus A_2 \oplus B_1 \oplus B_2. \end{aligned} \quad (62)$$

Similarly, we can obtain the basis polynomials for C_{2v} representation, which are listed in Table IV for $l \leq 2$.

In a typical lattice calculation, we can easily investigate is the A_1 sector. We will therefore concentrate on this sector. As is seen, up to $l \leq 2$, s -wave, p -wave and d -wave contribute to this sector. The other symmetry sectors can be easily worked out in the same way.

First, let us consider the angular momentum cutoff $\Lambda = 0$. From the reduction relations (61,62) and Tables III, IV, we note that only $\mathcal{M}_{00,00}^{\mathbf{d}}$ belongs to this sector, and Eq. (60) can be written as

$$\tan \delta_0(k) = \frac{1}{\mathcal{M}_{00,00}^{\mathbf{d}}} = \frac{\gamma q \pi^{3/2}}{\mathcal{Z}_{00}^{\mathbf{d}}(1; q^2)}, \quad q = \frac{L}{2\pi} k. \quad (63)$$

This is our essential result.

l	m	l'	m'	$M_{lm, l'm'}^{\mathbf{d}}$
0	0	0	0	w_{00}
1	0	0	0	iw_{10}
1	0	1	0	$w_{00} + 2w_{20}$
1	1	1	1	$w_{00} - w_{20}$
2	0	0	0	$-\sqrt{5}w_{20}$
2	0	1	0	$i\sqrt{\frac{4}{5}}w_{10}$
2	1	1	1	$i\sqrt{\frac{1}{5}}w_{10}$
2	0	2	0	$w_{00} + \frac{10}{7}w_{20}$
2	1	2	1	$w_{00} + \frac{5}{7}w_{20}$
2	2	2	-2	$\frac{3}{7}\sqrt{70}w_{44}$
2	2	2	2	$w_{00} - \frac{10}{7}w_{20} + \frac{3}{7}w_{40}$
3	0	0	0	$-iw_{30}$
3	0	1	0	$-\frac{3}{7}\sqrt{21}w_{20}$
3	1	1	1	$-\frac{3}{7}\sqrt{14}w_{20} + \frac{3}{7}\sqrt{14}w_{40}$
3	3	1	-1	$2\sqrt{3}w_{44}$
3	0	2	0	$-i3\sqrt{\frac{3}{35}}w_{10}$
3	1	2	1	$-i2\sqrt{\frac{6}{35}}w_{10}$
3	2	2	2	$i\sqrt{\frac{3}{7}}w_{10}$
3	0	3	0	$w_{00} + \frac{4}{3}w_{20}$
3	1	3	1	$w_{00} + w_{20}$
3	2	3	-2	$\frac{3}{11}\sqrt{70}w_{44}$
3	2	3	2	$w_{00} - \frac{21}{11}w_{40}$
3	3	3	-1	$\frac{3}{11}\sqrt{42}w_{44}$
3	3	3	3	$w_{00} - \frac{5}{3}w_{20} + \frac{9}{11}w_{40}$
				$+\frac{100}{33}w_{60} - \frac{25}{11}w_{60} + \frac{10}{11}\sqrt{14}w_{64} + \frac{10}{11}w_{60} - \frac{5}{33}\sqrt{210}w_{64} - \frac{5}{33}w_{60}$

TABLE I: The matrix elements $\mathcal{M}_{lm, l'm'}^{\mathbf{d}}$ for $\mathbf{d} = (0, 0, 1)$, $m_1 \neq m_2$ and $l, l' \leq 3$.

\mathbf{d}	point group	classification	N_{elements}
$(0, 0, 0)$	O_h	cubic	48
$(0, 0, a)$	C_{4v}	tetragonal	8
$(0, a, a)$	C_{2v}	orthorhombic	4

TABLE II: The categorizations of the boosts on a cubic box and its reduction of the cubic group. The first column shows the boost direction and a is a non-zero real number. Here we adopted the Schonflies notation [24].

If the angular momentum cutoff $\Lambda = 1$, we should take the sector $l = 1$ into consideration, and the matrix in Eq. (60) is two-dimensional. Hence, the determinant condition contains both phase shifts δ_0 and δ_1 ,

$$[e^{2i\delta_0}(m_{00} - i) - (m_{00} + i)] [e^{2i\delta_1}(m_{11} - i) - (m_{11} + i)] = m_{10}^2 (e^{2i\delta_0} - 1) (e^{2i\delta_1} - 1), \quad (64)$$

where we denote $m_{ab} \equiv \mathcal{M}_{a0, b0}^{\mathbf{d}}$. If $\delta_1 = 0 \pmod{\pi}$, as what we expected, Eq. (64) reduces nicely to Eq. (63). If $\delta_1 \neq 0$. Normally we can reasonably suppose that the lowest l -channel dominate the scattering phase. This is

representation	$l = 0$	$l = 1$	$l = 2$	indices
A_1	1	x_3	$x_3^2 - \frac{1}{3}x^2$	
A_2				
B_1			$x_1^2 - x_2^2$	
B_2			x_1x_2	
E		x_i	$x_i x_3$	$i = 1, 2$

TABLE III: The basis polynomials for the irreducible representations of C_{4v} .

quite right in the low-energy elastic scattering [2, 6].

If we expand $\delta_0 = \delta_0^0 + \Delta_0$, where δ_0^0 meets Eq. (63) and Δ_0 is a perturbative term, we can give the first order correction, namely,

$$\Delta_0(k) = \sigma(k)\delta_1(k).$$

The function $\sigma(k)$ stands for the sensitivity of the higher scattering phases. For C_{4v} symmetry, it is given by

$$\sigma(k) = -\frac{m_{10}^2}{m_{00}^2 + 1},$$

representation	$l = 0$	$l = 1$	$l = 2$
A_1	1	x_3	$x_3^2 - \frac{1}{3}x^2$
A_2			x_1x_2
B_1		x_1	x_1x_3
B_2		x_2	x_2x_3

TABLE IV: The basis polynomials for the irreducible representations of C_{2v} .

which is not usually small. To make sure that the Eq. (63) is a well approximation, the phase shift $\delta_1(k)(\text{mod}\pi)$ should be small. Fortunately, the physical case is often like this way: the elastic scattering is often dominated by the lowest l - channel.

The sensitivity function $\sigma(q^2)$ can be calculated using the matrix elements provided in Eq. (57) discussed in Appendices A and B. The sensitivity function $\sigma(q^2)$ for C_{4v} symmetry with $\alpha = 1.15$ and $\gamma = 1.177$ is illustrated in Fig. 1, here γ is a boost factor, and α -factor is defined in Eq. (50), which are typical values we used in Ref. [20]. In Fig. 1 the lower panel is the same sensitivity function as the upper panel just to display some detailed variations.

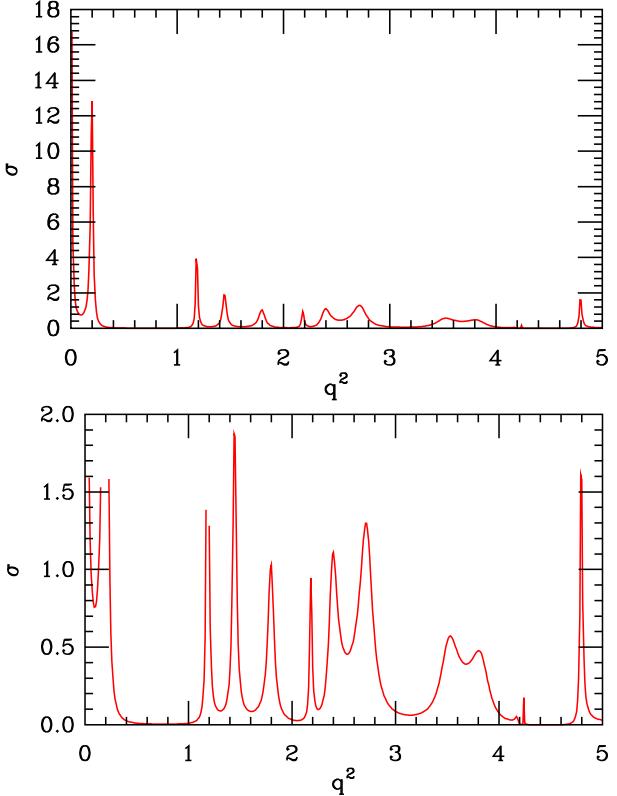


FIG. 1: The sensitivity $\sigma(q^2)$ for C_{4v} symmetry with parameters $\alpha = 1.15$ and $\gamma = 1.177$.

In the work, we also calculate the sensitivity function $\sigma(q^2)$ using the some typical α and γ values, we found

that it often varies in the range $0 - 20$, in Figs. 2, 3, and 4, we plotted just three of them. We can note that the sensitivity function $\sigma(q^2)$ is finite for all $q^2 > 0$. For some special values of q^2 , however, the sensitivity function $\sigma(q^2)$ has a sharp peak. For other values of q^2 away from these values, $\sigma(p^2)$ is always not too large.

We also note that, when $q \rightarrow 0$, the sensitivity function $\sigma(q^2)$ is often large. However, it does not usually cause any problem because it is nicely canceled out by δ_1 which is of q^3 order at small q [2, 6]. Thus, for the range $0 < q^2 < 1.1$ (except some special q^2 values), the Eq. (63) can be considered a good approximation. In fact, it is the range which are usually used to study the elastic scattering from lattice QCD [20].

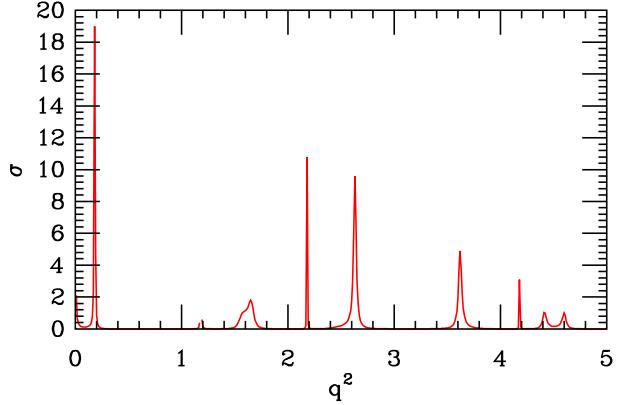


FIG. 2: The sensitivity $\sigma(q^2)$ for C_{4v} symmetry with parameters $\alpha = 1.05$ and $\gamma = 1.177$.

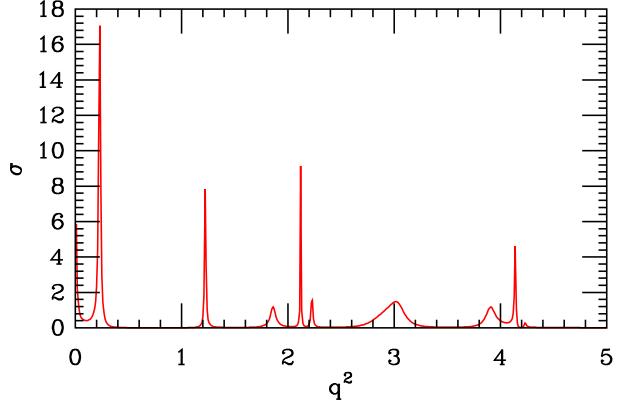


FIG. 3: The sensitivity $\sigma(q^2)$ for C_{4v} symmetry with parameters $\alpha = 1.1$ and $\gamma = 1.067$.

We should bear in mind that if $\delta_1(k)$ is not small, it is very difficult to extract the phase shift from energy spectrum [6]. In principle, we can still extract the s -wave scattering phase from Eq. (64) through dividing the p -wave phase shift by lattice simulations at various energy [6], because the corrections due to higher scattering

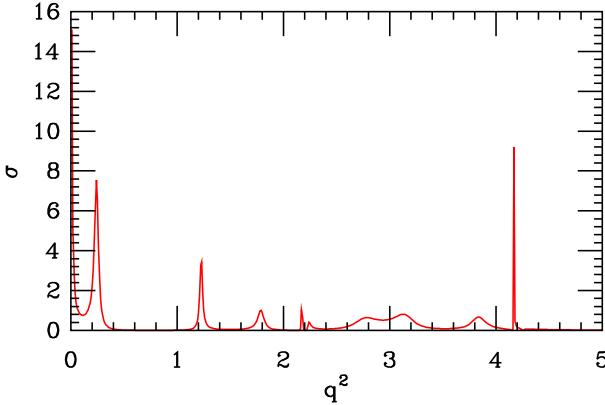


FIG. 4: The sensitivity $\sigma(q^2)$ for C_{4v} symmetry with parameters $\alpha = 1.15$ and $\gamma = 1.067$.

phases can also be estimated from lattice calculations. For example, from Table III, it is easily noted that, for lattices with C_{4v} symmetry, by inspecting energy eigenvalues of E symmetry, we can get an approximate estimate for the p -wave scattering phase δ_1 which dominates this symmetry sector. It seems to be too difficult, however naturally, it is still possible to calculate the energy spectrum, this is our future tasks.

If we choose the sector $\mathbf{d} = 0$, the moving and the CM frames coincide, $\gamma \rightarrow 1$ and $P_{\mathbf{d}} \rightarrow \mathbb{Z}^3$, and Eq. (64) nicely reduces to the form given in Ref. [2]. Of course, if we select $m_1 = m_2$ and $P_{\mathbf{d}} \rightarrow \{\mathbf{r} \in \mathbf{R}^3 \mid \mathbf{r} = \vec{\gamma}^{-1}(\mathbf{n} + \mathbf{d}/2)\}$, $\mathbf{n} \in \mathbb{Z}^3$, and Eq. (64) neatly reduces to the form presented in Ref. [6]. These are what we expected.

As for $\Lambda = 2$ or higher, it is quite complicated. See the relevant discussions in Ref. [7]. Bearing in mind that this work is an exploratory study for some systems like the πK system, the main purpose is to present some conceptual and theoretical issues.

V. CONCLUSION

In the current work we have strictly investigated the scattering states of two-particle with unequal mass, and the best-efforts are paid to derive the modified \mathbf{d} -periodic rule which is crucial to the alteration of the Rummukainen-Gottlieb's formula. The finite size expressions, which can be regarded as a generalization of the Rummukainen-Gottlieb's formulae to the generic two-particle system in the moving frame, are developed. We also checked that all the Rummukainen-Gottlieb's results in Ref. [6] is nicely restored if we set $m_1 = m_2$.

Since the so-called κ meson is a low-lying scalar meson with strangeness, a study of κ meson decay is an explicit exploration of the three-flavor structure of the low-energy hadronic interactions, which is not directly probed in $\pi\pi$ scattering, therefore, it is a significant step for us under-

standing the dynamical aspect of hadron reactions with QCD. Moreover, BES collaboration recently carried out some experimental measurements [25, 26] to investigate κ resonance mass and its decay width. With the modified formula in Eq. (63) and our strict discussion of this formula from theoretical aspects, now it will be possible to compute the resonance masses and perhaps its decay widths of some resonances including possible exotic hadrons as well as traditional hadrons like κ and vector kaon K^* , etc., directly from lattice simulation in a correct manner. We have already used these formulae to preliminarily analyze our πK scattering at $I = 1/2$ channel [20], and the reasonable results of our lattice simulation data supports these formula.

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Appendix A: The calculation of zeta function

The method for evaluating the zeta function for $\mathbf{d} = 0$ has been discussed by Lüscher in Ref. [2]. Rummukainen and Gottlieb extended this discussion in the MF for $\mathbf{d} \neq 0, \alpha = 1$ [6]. The formalism used here is further adapted to the case of $\mathbf{d} \neq 0, \alpha \neq 1$, and we just present the essential formulae.

We first denotes the heat kernel on a modified \mathbf{d} -periodic torus in Eq. (48), namely,

$$K_{\mathbf{d}}(t, \mathbf{x}) = \frac{1}{(2\pi)^3} \sum_{\mathbf{r} \in P_{\mathbf{d}}} e^{i\mathbf{r} \cdot \mathbf{x} - t\mathbf{r}^2} \quad (\text{A1})$$

where the summation for \mathbf{r} is carried out over the set

$$P_{\mathbf{d}} = \left\{ \mathbf{r} \mid \mathbf{r} = \vec{\gamma}^{-1} \left(\mathbf{n} + \frac{\alpha}{2} \mathbf{d} \right), \quad \mathbf{n} \in \mathbb{Z}^3 \right\}, \quad (\text{A2})$$

here the factor α is denoted in Eq. (50), and the operation $\vec{\gamma}^{-1}$ is defined in Eq. (4). Following from Poisson's identity, we can rewrite the heat kernel as

$$K_{\mathbf{d}}(t, \mathbf{x}) = \gamma \frac{1}{(4\pi t)^{\frac{3}{2}}} e^{i1/2\alpha\mathbf{d} \cdot \mathbf{x}} \times \sum_{\mathbf{n} \in \mathbb{Z}^3} e^{-i\alpha\pi\mathbf{d} \cdot \mathbf{n}} \exp \left[-\frac{1}{4t} (\mathbf{x} - 2\pi\vec{\gamma} \mathbf{n})^2 \right]. \quad (\text{A3})$$

The expression in Eq. (A1) is fast convergent for large t , and the expression in Eq. (A3) is useful for small t . We can denote the truncated heat kernel $K_{\mathbf{d}}^{\lambda}(t, \mathbf{x})$ by

$$K_{\mathbf{d}}^{\lambda}(t, \mathbf{x}) = K_{\mathbf{d}}(t, \mathbf{x}) - \sum_{\mathbf{r} \in P_{\mathbf{d}}, |\mathbf{r}| > \lambda} \exp(i\mathbf{r} \cdot \mathbf{x} - t\mathbf{r}^2).$$

We apply the operator $\mathcal{Y}_{lm}(-i\nabla_{\mathbf{x}})$ to heat kernels,

$$\mathcal{K}_{\mathbf{d},lm}^{\lambda}(t, \mathbf{x}) = \mathcal{Y}_{lm}(-i\nabla_{\mathbf{x}})\mathcal{K}_{\mathbf{d}}^{\lambda}(t, \mathbf{x}). \quad (\text{A4})$$

We can easily show that the zeta function has a rapidly convergent integral expression

$$\begin{aligned} \mathcal{Z}_{lm}^{\mathbf{d}}(1; q^2) &= \sum_{\mathbf{r} \in P_{\mathbf{d}}, |\mathbf{r}| < \lambda} \frac{\mathcal{Y}_{lm}(\mathbf{r})}{\mathbf{r}^2 - q^2} \\ &+ (2\pi)^3 \int_0^\infty dt \left(e^{tq^2} K_{\mathbf{d},lm}^{\lambda}(t, \mathbf{0}) - \frac{\gamma \delta_{l,0} \delta_{m,0}}{16\pi^2 t^{3/2}} \right). \end{aligned} \quad (\text{A5})$$

To calculate the integrand, we use the Eq. (A1) when $t \geq 1$, and the Eq. (A3) in the case of $t < 1$. The cutoff λ is chosen such that $\lambda^2 > \text{Re } q^2$. We can easily verify that, when $m_1 = m_2$ (or equivalently $\alpha = 1$), the Rummukainen-Gottlieb's result in Ref. [6] is restored.

Appendix B: The evaluation of the zeta function

$$\mathcal{Z}_{10}(s; q^2)$$

In this appendix we briefly discuss one useful method for numerical evaluation of zeta function $\mathcal{Z}_{10}(s; q^2)$. Here

we follow the methods and notations in Ref. [11].

The definition of the zeta function $\mathcal{Z}_{10}^{\mathbf{d}}(s; q^2)$ in Eq. (56) is

$$\sqrt{\frac{4\pi}{3}} \cdot \mathcal{Z}_{10}^{\mathbf{d}}(s; q^2) = \sum_{\mathbf{r} \in P_{\mathbf{d}}} \frac{r_3}{(r^2 - q^2)^s}, \quad (\text{B1})$$

where the summation for \mathbf{r} is carried out over the set

$$P_{\mathbf{d}} = \left\{ \mathbf{r} \mid \mathbf{r} = \vec{\gamma}^{-1} \left(\mathbf{n} + \frac{\alpha}{2} \mathbf{d} \right), \quad \mathbf{n} \in \mathbb{Z}^3 \right\}, \quad (\text{B2})$$

here the factor α is denoted in Eq. (50). The operation $\vec{\gamma}^{-1}$ is defined in Eq. (4). We consider that the value q^2 can be a positive or negative.

First we consider the case of $q^2 > 0$, and we can separate the summation in $\mathcal{Z}_{10}^{\mathbf{d}}(s; q^2)$ into two parts as

$$\sum_{\mathbf{r} \in P_{\mathbf{d}}} \frac{r_3}{(r^2 - q^2)^s} = \sum_{r^2 < q^2} \frac{r_3}{(r^2 - q^2)^s} + \sum_{r^2 > q^2} \frac{r_3}{(r^2 - q^2)^s}. \quad (\text{B3})$$

The second term can be written in an integral form,

$$\begin{aligned} \sum_{r^2 > q^2} \frac{r_3}{(r^2 - q^2)^s} &= \frac{1}{\Gamma(s)} \sum_{r^2 > q^2} r_3 \left[\int_0^1 dt t^{s-1} e^{-t(r^2 - q^2)} + \int_1^\infty dt t^{s-1} e^{-t(r^2 - q^2)} \right] \\ &= \frac{1}{\Gamma(s)} \int_0^1 dt t^{s-1} e^{tq^2} \sum_{\mathbf{r}} r_3 e^{-r^2 t} - \sum_{r^2 < q^2} \frac{r_3}{(r^2 - q^2)^s} + \sum_{\mathbf{r}} r_3 \frac{e^{-(r^2 - q^2)}}{(r^2 - q^2)^s}. \end{aligned} \quad (\text{B4})$$

The second term neatly cancel out the first term in Eq. (B3). Using Poisson's resummation formula we can rewrite the first term in Eq. (B4) as

$$\begin{aligned} \frac{1}{\Gamma(s)} \int_0^1 dt t^{s-1} e^{tq^2} \sum_{\mathbf{r}} r_3 e^{-r^2 t} &= \frac{\sqrt{\pi}}{\Gamma(s)} \int_0^1 dt t^{s-1} e^{tq^2} \left(\frac{\pi}{t} \right)^2 \sum_{\mathbf{n} \in \mathbb{Z}^3} i n_3 e^{-i\alpha\pi\mathbf{n} \cdot \mathbf{d}} e^{-(\pi\vec{\gamma}\mathbf{n})^2/t} \\ &= \frac{\sqrt{\pi}}{\Gamma(s)} \int_0^1 dt t^{s-1} e^{tq^2} \left(\frac{\pi}{t} \right)^2 \sum_{\mathbf{n} \in \mathbb{Z}^3} n_3 \sin(\alpha\pi\mathbf{n} \cdot \mathbf{d}) e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}, \end{aligned} \quad (\text{B5})$$

where the imaginary parts are neatly canceled out.

After gathering all terms we obtain the zeta function at $s = 1$ as,

$$\begin{aligned} \sqrt{\frac{4\pi}{3}} \cdot \mathcal{Z}_{10}^{\mathbf{d}}(1; q^2) &= \sum_{\mathbf{r} \in P_{\mathbf{d}}} r_3 \frac{e^{-(r^2 - q^2)}}{r^2 - q^2} + \\ &\sqrt{\pi} \int_0^1 dt e^{tq^2} \left(\frac{\pi}{t} \right)^2 \sum_{\mathbf{n} \in \mathbb{Z}^3} n_3 \sin(\alpha\pi\mathbf{n} \cdot \mathbf{d}) e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}. \end{aligned} \quad (\text{B6})$$

For the case of $q^2 \leq 0$, it is not necessary for us to separate the summation in $\mathcal{Z}_{10}(s; q^2)$, and it can be also written in an integral form. Following the same procedures, we arrive at the same expression in Eq. (B6).

Hence, Eq. (B6) can be applied for both cases.

Substituting $\mathbf{d} = (0, 0, 1)$ into Eq. (B6) we obtain the zeta function in Eq. (56)

$$\begin{aligned} \sqrt{\frac{4\pi}{3}} \cdot \mathcal{Z}_{10}^{\mathbf{d}}(1; q^2) &= \sum_{\mathbf{r} \in P_{\mathbf{d}}} r_3 \frac{e^{-(r^2 - q^2)}}{r^2 - q^2} + \\ &\sqrt{\pi} \int_0^1 dt e^{tq^2} \left(\frac{\pi}{t} \right)^2 \sum_{\mathbf{n} \in \mathbb{Z}^3} n_3 \sin(\alpha\pi n_3) e^{-(\pi\vec{\gamma}\mathbf{n})^2/t}. \end{aligned} \quad (\text{B7})$$

We can easily verify that, if $m_1 = m_2$, zeta function $\mathcal{Z}_{10}(1; q^2) \rightarrow 0$, the Rummukainen-Gottlieb's result is recovered.

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